

Implications of Poincaré symmetry for thermal field theories in finite-volume

Leonardo Giusti

*Dipartimento di Fisica, Università di Milano–Bicocca,
and INFN, sezione di Milano–Bicocca,
I-20126 Milano, Italy
Leonardo.Giusti@mib.infn.it*

Harvey B. Meyer

*PRISMA Cluster of Excellence,
Institut für Kernphysik and Helmholtz Institute Mainz
Johannes Gutenberg-Universität Mainz
D-55099 Mainz, Germany
meyerh@kph.uni-mainz.de*

ABSTRACT: The analytic continuation to an imaginary velocity $i\xi$ of the canonical partition function of a thermal system expressed in a moving frame has a natural implementation in the Euclidean path-integral formulation in terms of shifted boundary conditions. Writing the Boltzmann factor as $\exp[-L_0(\hat{H} - i\xi \cdot \hat{\mathbf{P}})]$, the Poincaré invariance underlying a relativistic theory implies a dependence of the free-energy on L_0 and the shift ξ only through the combination $\beta = L_0\sqrt{1 + \xi^2}$. This in turn implies a set of Ward identities, some of which were previously derived by us, among the correlators of the energy-momentum tensor. In the infinite-volume limit they lead to relations among the cumulants of the total energy distribution and those of the momentum, i.e. they connect the energy and the momentum distributions in the canonical ensemble. In finite volume the Poincaré symmetry translates into exact relations among partition functions and correlation functions defined with different sets of (generalized) periodic boundary conditions. They have interesting applications in lattice field theory. In particular, they offer Ward identities to renormalize non-perturbatively the energy-momentum tensor and novel ways to compute thermodynamic potentials. At fixed bare parameters they also provide a simple method to vary the temperature in much smaller steps than with the standard procedure.

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1. Introduction

It is a recurring theme in quantum field theory that a symmetry has far reaching consequences even when it is softly broken¹. In this paper we show that, for a relativistic theory set up on a space with one or more dimensions of finite length and (generalized) periodic boundary conditions², the underlying Lorentz symmetry leads to interesting consequences.

¹Here with “softly” we refer to any breaking which does not modify the renormalization pattern of the theory, e.g. mass terms and (generalized) periodic boundary conditions.

²Translational invariance is thus preserved.

When continued analytically to an imaginary velocity vector $\mathbf{v} = i\boldsymbol{\xi}$, where $\boldsymbol{\xi} \in \mathbb{R}^3$, the canonical partition function of a thermal field theory formulated in a moving frame has a straightforward definition in the functional integral formalism. It is the ordinary Euclidean path integral with shifted boundary conditions in the time-direction [1, 2]. In the zero-temperature limit and in presence of a mass gap, the invariance of the theory (and of its vacuum) under the Poincaré group forces its free-energy to be independent of the shift $\boldsymbol{\xi}$. At non-zero temperature the finite time-length L_0 breaks the euclideanized Lorentz group softly, consequently the free energy depends on the shift (velocity) explicitly but only through the combination $\beta = L_0 \sqrt{1 + \boldsymbol{\xi}^2}$. An interesting set of Ward identities (WIs) follows. As shown in section 2, they provide a recursion relation among the cumulants of the momentum distribution [1, 2], they relate the total energy and momentum distributions in the rest-frame, and they suggest new ways to compute thermodynamic potentials. These results generalize those found in Ref. [2] to a generic theory and to a generic value of the shift $\boldsymbol{\xi}$. For the clarity of the presentation and to avoid unessential technical complications, however, we restrict ourselves to bosonic theories in this paper.

The considerations above extend to a thermal theory set up in a finite spatial volume with periodic boundary conditions. The independence of the free energy on the angle between the time and the space directions is replaced by relations among partition functions of systems with the time and the spatial extensions L_k Lorentz transformed, e.g.

$$Z(L_0, L_1, L_2, L_3; \xi_1) = Z\left(\frac{L_1}{\sqrt{1 + \xi_1^2}}, L_0 \sqrt{1 + \xi_1^2}, L_2, L_3; -\xi_1\right) \quad (1.1)$$

with $\boldsymbol{\xi} = (\xi_1, 0, 0)$. The WIs are readily extended to finite-volume systems.

These properties find interesting applications when a theory is discretized on the lattice, where a non-zero shift can easily be implemented [1]. Lorentz invariance, which is recovered in the continuum limit only, allows one to vary the temperature of the system by changing either $\boldsymbol{\xi}$ or L_0 , i.e. in much *smaller* steps (at fixed bare parameters) with respect to varying L_0 alone. Thanks to the misalignment of the lattice axes with respect to the periodic directions, the WIs provide new ways to compute thermodynamic potentials numerically and new conditions to renormalize non-perturbatively the energy-momentum tensor.

2. Thermal field theory in a moving frame

In this section we focus on properties of a relativistic thermal system in the infinite-volume limit. In a moving frame, the total energy and momentum densities are given by ([3], paragraph 133)

$$e' = \frac{1}{1 - \mathbf{v}^2} (e + \mathbf{v}^2 p), \quad \mathbf{p}' = \frac{e + p}{1 - \mathbf{v}^2} \mathbf{v}, \quad (2.1)$$

where \mathbf{v} is the velocity of the center-of-mass relative to the observer, e and p are the energy density and pressure in the rest frame respectively. The enthalpy density $(e + p)$ in the rest frame plays the role of the inertial mass density of the system, and its rest volume appears contracted by a factor $\sqrt{1 - \mathbf{v}^2}$ in the moving frame. The standard definition of

the partition function is³ ([4], paragraph 2)

$$\mathcal{Z}(L_0, \mathbf{v}) \equiv \text{Tr} \{ e^{-L_0(\hat{H} - \mathbf{v} \cdot \hat{\mathbf{P}})} \} , \quad (2.2)$$

where \hat{H} and $\hat{\mathbf{P}}$ are the Hamiltonian and the total momentum operator expressed in a moving frame. We focus on the Euclidean formulation, where it is natural to continue \mathcal{Z} to imaginary velocities $\mathbf{v} = i\boldsymbol{\xi}$ with the Lorentz group replaced by $\text{SO}(4)$. The partition function

$$Z(L_0, \boldsymbol{\xi}) = \text{Tr} \{ e^{-L_0(\hat{H} - i\boldsymbol{\xi} \cdot \hat{\mathbf{P}})} \} \quad (2.3)$$

corresponds to the ordinary Euclidean path integral with shifted boundary conditions in the time-direction [1, 2]. The free-energy density can be defined as usual

$$f(L_0, \boldsymbol{\xi}) = -\frac{1}{L_0 V} \ln Z(L_0, \boldsymbol{\xi}) , \quad (2.4)$$

where V is the volume observed in the moving frame. In the thermodynamic limit the invariance of the dynamics under the $\text{SO}(4)$ group implies

$$f(L_0, \boldsymbol{\xi}) = f(L_0 \sqrt{1 + \boldsymbol{\xi}^2}, \mathbf{0}) . \quad (2.5)$$

In section 4 we derive this equation in the path integral formalism starting from a finite-volume system, and provide the functional form for the finite-volume corrections. Eq. (2.5) is consistent with modern thermodynamic arguments on the Lorentz transformation of the temperature and the free energy [5, 6] (the issue has been debated for a long time, see [7] for a recent discussion). Before entering into the details of the derivation it is interesting to discuss the origin of this formula, and to anticipate some of the implications of the rich kinematics in the boundary conditions that Lorentz symmetry allows for in the path-integral formulation.

2.1 Ward identities for the total energy and momentum

Relation (2.5) is the source of certain WIs for the energy-momentum tensor, some of which were already derived in Ref. [1, 2]. They can be generated in a quasi-automated fashion by deriving the free-energy density with respect to L_0 and ξ_k . By remembering that the cumulants of the total momentum distribution can be written as [1]

$$k_{\{2n_1, 2n_2, 2n_3\}} \equiv \frac{1}{V} \langle \hat{P}_1^{2n_1} \hat{P}_2^{2n_2} \hat{P}_3^{2n_3} \rangle_c = \frac{(-1)^{n_1+n_2+n_3+1}}{L_0^{2n_1+2n_2+2n_3-1}} \frac{\partial^{2n_1}}{\partial \xi_1^{2n_1}} \frac{\partial^{2n_2}}{\partial \xi_2^{2n_2}} \frac{\partial^{2n_3}}{\partial \xi_3^{2n_3}} f(L_0, \boldsymbol{\xi}) \Big|_{\boldsymbol{\xi}=0} , \quad (2.6)$$

in the thermodynamic limit a plethora of Ward identities among on-shell correlators of the total momentum and/or energy are derived by inserting Eq. (2.5) in (2.6). By choosing $\boldsymbol{\xi} = \{\xi_1, 0, 0\}$, it is straightforward to derive the master equation

$$\frac{k_{\{2n, 0, 0\}}}{L_0} = (-1)^{n+1} (2n-1)!! \left\{ \frac{1}{L_0} \frac{\partial}{\partial L_0} \right\}^n f(L_0, \boldsymbol{\xi}) \Big|_{\boldsymbol{\xi}=0} \quad n = 1, 2, \dots \quad (2.7)$$

³We use the notation L_0 because this parameter represents the length of the Euclidean time direction in the path integral formalism.

If we remember that in the Euclidean the momentum operator maps to $\hat{P}_k \rightarrow -i\bar{T}_{0k}$, where $\bar{T}_{\mu\nu}(x_0) = \int d^3x T_{\mu\nu}(x)$ with $T_{\mu\nu}$ being the energy-momentum field of the theory, an immediate consequence of Eq. (2.7) is the recursion relation (x_0^i all different)

$$\langle \bar{T}_{01}(x_0^1) \dots \bar{T}_{01}(x_0^{2n}) \rangle_c = (2n-1) \frac{\partial}{\partial L_0} \left\{ \frac{1}{L_0} \langle \bar{T}_{01}(x_0^3) \dots \bar{T}_{01}(x_0^{2n}) \rangle_c \right\} \quad n = 2, 3, \dots \quad (2.8)$$

which extends to a generic theory the derivation presented for the scalar one in Ref. [2]. Cumulants with non-null indices in the other directions can be related to those in (2.7) by cubic symmetry.

If we define $c_1 \equiv e - f$ and recall that the higher cumulants of the total energy distribution are given by

$$c_n \equiv \frac{1}{V} \langle \hat{H}^n \rangle_c = (-1)^{n+1} \left[n \frac{\partial^{n-1}}{\partial L_0^{n-1}} + L_0 \frac{\partial^n}{\partial L_0^n} \right] f(L_0, \xi) \Big|_{\xi=0} \quad n = 2, 3, \dots, \quad (2.9)$$

it is clear that there is a linear relation among c_1, \dots, c_n and the n first derivatives of the free-energy density. Since Eq. (2.7) gives the $k_{\{2n,0,0\}}$ as linear combinations of the very same derivatives, a linear relation exists among the n first non-trivial cumulants of the energy and momentum distributions in the thermodynamic limit. Some details of the required combinatorics are summarized in appendix A. The result reads⁴

$$k_{\{2n,0,0\}} = \frac{(2n-1)!!}{(2L_0^2)^n} \sum_{\ell=1}^n \frac{(2n-\ell)!}{\ell!(n-\ell)!} (2L_0)^\ell c_\ell, \quad (2.10)$$

and it shows that the total energy and momentum distributions of a relativistic thermal theory are related. Up to $n = 4$ we obtain

$$\begin{aligned} L_0 k_{\{2,0,0\}} &= c_1, \\ L_0^3 k_{\{4,0,0\}} &= 9 c_1 + 3 L_0 c_2, \\ L_0^5 k_{\{6,0,0\}} &= 225 c_1 + 90 L_0 c_2 + 15 L_0^2 c_3, \\ L_0^7 k_{\{8,0,0\}} &= 11025 c_1 + 4725 L_0 c_2 + 1050 L_0^2 c_3 + 105 L_0^3 c_4. \end{aligned} \quad (2.11)$$

As expected $c_1 = e + p$ is necessarily positive. Since $L_0^2 c_2$ is the specific heat, the fourth cumulant of the momentum turns out to always be positive. If we remember that in the Euclidean $\langle T_{00} \rangle = -e$ and $\langle T_{kk} \rangle = p$, Eqs. (2.11) can also be written as

$$\begin{aligned} L_0 \langle \bar{T}_{01} T_{01} \rangle_c &= \langle T_{00} \rangle - \langle T_{11} \rangle, \\ L_0^3 \langle \bar{T}_{01} \bar{T}_{01} \bar{T}_{01} T_{01} \rangle_c &= 9 \langle T_{11} \rangle - 9 \langle T_{00} \rangle + 3 L_0 \langle \bar{T}_{00} T_{00} \rangle_c, \\ &\dots \end{aligned} \quad (2.12)$$

where in each correlator the energy-momentum fields are inserted at different times. These WIs generalize to all cumulants of a generic field theory those found in Refs. [1, 2]. They show that the thermodynamics of a relativistic theory can be studied from its thermal momentum distribution and vice-versa.

⁴Notice that the coefficients multiplying c_ℓ are all positive.

2.2 Ward identities in presence of a non-zero shift

When $\xi \neq 0$ parity is softly broken by the boundary conditions in the compact direction, odd derivatives in the ξ_k do not vanish anymore, and new interesting WIs hold. By deriving once with respect to L_0 and ξ_k , it is easy to obtain the first non-trivial relation

$$\langle T_{0k} \rangle_{\xi} = \frac{\xi_k}{1 - \xi_k^2} \{ \langle T_{00} \rangle_{\xi} - \langle T_{kk} \rangle_{\xi} \} . \quad (2.13)$$

An interesting consequence of this equation is that the entropy density s of the system at the inverse temperature $\beta = L_0 \sqrt{1 + \xi^2}$ is given by

$$s = - \frac{L_0}{\gamma^3 \xi_k} \langle T_{0k} \rangle_{\xi} \quad (2.14)$$

which, by following Refs. [1, 2], can also be written as

$$s = - \frac{1}{V \gamma^3 \xi_k} \frac{\partial}{\partial \xi_k} \ln Z(L_0, \xi) \quad (2.15)$$

where $\gamma = 1/\sqrt{1 + \xi^2}$. Ward identities among correlators with more fields can easily be obtained by considering higher order derivatives in L_0 and ξ_k . For instance by deriving two times with respect to the shift components, by using

$$L_0 \langle \bar{T}_{0k}(L_0) O \rangle_{\xi, c} = \frac{\partial}{\partial \xi_k} \langle O \rangle_{\xi} \quad (2.16)$$

where O is a generic field with support located at a physical distance from the time-slice L_0 , we obtain

$$\langle T_{0k} \rangle_{\xi} = \frac{L_0 \xi_k}{2} \sum_{ij} \langle \bar{T}_{0i} T_{0j} \rangle_{\xi, c} \left[\delta_{ij} - \frac{\xi_i \xi_j}{\xi^2} \right] . \quad (2.17)$$

This equation and Eq. (2.13) can be enforced in regularizations that break translational invariance, such as the lattice, to renormalize non-perturbatively the traceless components of the energy-momentum tensor, see section 5. By combining Eqs. (2.14) and (2.17), the entropy density can also be computed as

$$s^{-1} = - \frac{\gamma^3}{2} \sum_{ij} \frac{\langle \bar{T}_{0i} T_{0j} \rangle_{\xi, c}}{\langle T_{0i} \rangle_{\xi} \langle T_{0j} \rangle_{\xi}} \xi_i \xi_j \left[\delta_{ij} - \frac{\xi_i \xi_j}{\xi^2} \right] , \quad (2.18)$$

and the analogous expression for the specific heat reads

$$\frac{c_v}{s^2} = - \frac{\gamma^3}{2} \sum_{ij} \frac{\langle \bar{T}_{0i} T_{0j} \rangle_{\xi, c}}{\langle T_{0i} \rangle_{\xi} \langle T_{0j} \rangle_{\xi}} \frac{\xi_i \xi_j}{\xi^2} \left[(1 - 2\xi^2) \delta_{ij} - 3 \frac{\xi_i \xi_j}{\xi^2} \right] . \quad (2.19)$$

3. Generalized periodic boundary conditions

Consider a quantum field theory⁵ defined on \mathbb{R}^d , an orthonormal basis, and d linearly independent *primitive vectors* $v^{(\mu)}$ ($\mu = 0, 1, \dots, d-1$). The latter can be represented by a *primitive matrix* $V \in \text{GL}(d, \mathbb{R})$ whose columns are the components of $v^{(\mu)}$ in the orthonormal basis. For a given point labeled with the coordinates x_μ , the field is identified at all points with coordinates

$$x_\mu + V_{\mu\nu} m_\nu, \quad m_\nu \in \mathbb{Z}, \quad (3.1)$$

i.e. we impose generalized periodic boundary conditions (GPBCs)⁶. The shifted boundary conditions which implement the partition function in Eq. (2.3) are a special case of GPBCs.

In addition to the parameters already present in infinite volume, the finite-volume theory contains d^2 extra parameters specifying the coordinates of the primitive vectors. By defining the primitive cell as usual

$$\Omega = \left\{ x \in \mathbb{R}^d \mid x_\mu = V_{\mu\nu} t_\nu, \ 0 \leq t_\mu < 1 \right\}, \quad (3.2)$$

$d(d-1)/2$ parameters specify the orientation of the cell relative to the orthonormal basis (in $d=3$ and for orthogonal primitive vectors, these are the Euler angles), while $d(d+1)/2$ fix its geometry, namely the length of the vectors $v^{(\mu)}$ and the $d(d-1)/2$ angles between them. For a Lorentz-invariant theory, the absolute orientation of the primitive cell is clearly of no consequence. The partition function of the finite-volume theory is unchanged if V is replaced by

$$V \rightarrow \Lambda V, \quad \Lambda \in \text{SO}(d), \quad (3.3)$$

i.e. the $d(d-1)/2$ parameters that specify the orientation of the cell are redundant. This is the invariance which allows one to generalize Eq. (2.5) in finite volume, and to derive the corresponding WIs. At variance with the infinite-volume case, the partition function of a finite-volume theory is also left unchanged under the discrete group of transformations $\text{SL}(d, \mathbb{Z})$. As is well known from crystallography, two geometrically different primitive cells may in fact describe the same crystal: any set of vectors $v^{(\mu)}$ that generates the same discrete set of points where the fields are identified is equivalent. This amounts to the freedom of replacing the matrix V by a new matrix whose columns are linear combinations with integer coefficients of the columns of V , with the restriction that the inverse relation exists and contains only integer coefficients. The latter condition requires the determinant of the two primitive matrices to be equal up to a sign. Here we restrict ourselves to the transformations with positive sign, which maintain the orientation of the unit cell. In short, the transformation is

$$V \rightarrow VM, \quad M \in \text{SL}(d, \mathbb{Z}), \quad (3.4)$$

i.e. a discrete equivalence between two GPBCs. To summarize, the most general relation between two primitive matrices V and W corresponding to a relativistic field theory with

⁵Since the considerations in this section are valid for a generic number of dimensions $d > 1$, we leave the value of d unspecified. In the rest of the paper the results of this section will be used for $d=4$.

⁶For brevity we refer to a theory satisfying GPBCs as a finite-volume theory.

two different sets of GPBCs and equal partition functions, is given by

$$W = \Lambda V M, \quad \Lambda \in \text{SO}(d), \quad M \in \text{SL}(d, \mathbb{Z}) . \quad (3.5)$$

The matrix M modifies the geometry of the primitive cell, while Λ modifies its orientation. The freedom to choose the former is a property of periodic boundary conditions, the freedom to choose the latter is a property of the $\text{SO}(d)$ invariance of the infinite-volume field theory. The relation (3.5) defines an equivalence relation (in the mathematical sense) between the primitive matrices V and W . We will write the relation $V \sim W$. In Appendix B we verify in momentum space that two partition functions defined by path integrals with a common Lagrangian density and with equivalent sets of boundary conditions are equal. More precisely, the actions in the two theories are related by

$$S(V; [\phi]) = S(\Lambda V M; [\phi^\Lambda]), \quad (3.6)$$

where $[\phi^\Lambda]$ means that every field of the theory has been rotated. Correlation functions of fields can also be mapped between equivalent descriptions of the same system by taking into account their transformation properties under the $\text{SO}(d)$ group. It is also interesting to notice that, by an appropriate field transformation, the effect of the non-orthogonality of the original primitive vectors can be re-absorbed into a re-definition of the action, see again appendix B.

4. Finite-volume theory with shifted boundary conditions

The finite-volume analogue of the partition function⁷ (2.3)

$$Z(V_{\text{sbc}}) = \text{Tr} \{ e^{-L_0(\hat{H} - i\boldsymbol{\xi} \cdot \hat{\mathbf{P}})} \} , \quad (4.1)$$

where

$$V_{\text{sbc}} = \begin{pmatrix} L_0 & 0 & 0 & 0 \\ L_0 \xi_1 & L_1 & 0 & 0 \\ L_0 \xi_2 & 0 & L_2 & 0 \\ L_0 \xi_3 & 0 & 0 & L_3 \end{pmatrix} , \quad (4.2)$$

can be expressed as a Euclidean path integral with the fields satisfying standard periodic boundary conditions in the spatial directions, and shifted boundary conditions [1, 8] in time⁸

$$\phi(L_0, \mathbf{x}) = \phi(0, \mathbf{x} - L_0 \boldsymbol{\xi}) . \quad (4.3)$$

Due to the spatial periodicity, $\xi'_k = \xi_k + L_k/L_0$ is equivalent to ξ_k , and therefore the imaginary velocity components can be restricted to the interval

$$-\frac{L_k}{2L_0} < \xi_k \leq \frac{L_k}{2L_0} . \quad (4.4)$$

⁷In finite volume we will use the primitive matrix as argument of the partition function Z and of the free-energy f .

⁸Relative to these references, we adopt here a different sign convention for the shift in the path integral.

For later use it is useful to note the effect of taking derivatives of the partition function with respect to the external parameters,

$$\begin{aligned}
\langle T_{00} \rangle_{V_{\text{sbc}}} &= \frac{1}{L_0 L_1 L_2 L_3} \left(L_0 \frac{\partial}{\partial L_0} - \sum_k \xi_k \frac{\partial}{\partial \xi_k} \right) \ln Z(V_{\text{sbc}}) \\
\langle T_{0k} \rangle_{V_{\text{sbc}}} &= \frac{1}{L_0 L_1 L_2 L_3} \frac{\partial}{\partial \xi_k} \ln Z(V_{\text{sbc}}) \quad k = 1, 2, 3 \\
\langle T_{kk} \rangle_{V_{\text{sbc}}} &= \frac{1}{L_0 L_1 L_2 L_3} \left(L_k \frac{\partial}{\partial L_k} + \xi_k \frac{\partial}{\partial \xi_k} \right) \ln Z(V_{\text{sbc}}) \quad k = 1, 2, 3,
\end{aligned} \tag{4.5}$$

and to introduce the notation

$$\gamma = (1 + \boldsymbol{\xi}^2)^{-1/2}, \quad \gamma_{kl} = (1 + \xi_k^2 + \xi_l^2)^{-1/2}, \quad \gamma_k = (1 + \xi_k^2)^{-1/2}. \tag{4.6}$$

By defining

$$V_1 = M^{-1} R V_{\text{sbc}} M = \begin{pmatrix} L_1 \gamma_1 & 0 & 0 & 0 \\ -L_1 \gamma_1 \xi_1 & L_0 / \gamma_1 & 0 & 0 \\ 0 & L_0 \xi_2 & L_2 & 0 \\ 0 & L_0 \xi_3 & 0 & L_3 \end{pmatrix} \tag{4.7}$$

with

$$R = \begin{pmatrix} \gamma_1 & \gamma_1 \xi_1 & 0 & 0 \\ -\gamma_1 \xi_1 & \gamma_1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad M = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{4.8}$$

we conclude from section 3 that $Z(V_{\text{sbc}}) = Z(V_1)$. We first focus on the case $\xi_2 = \xi_3 = 0$, and later use the $\text{SO}(3)$ rotation symmetry to generalize the result to a generic shift vector. The partition function can be interpreted in terms of the states that propagate in the direction given by the first column of V_1 . In the thermal field theory language, the latter are the eigenstates of the ‘screening’ Hamiltonian \tilde{H} , which acts on states living on a slice of dimensions $(L_0 / \gamma_1) \times L_2 \times L_3$ with ordinary periodic boundary conditions. Their spectrum yields the spatial correlation lengths of the thermal system at inverse temperature (L_0 / γ_1) . The partition function can thus be written as

$$Z(V_1) = \text{Tr} \left\{ \exp -L_1 \gamma_1 (\tilde{H} + i \xi_1 \tilde{\omega}) \right\}, \tag{4.9}$$

where $\tilde{\omega}$ is the momentum operator along the primitive vector of length (L_0 / γ_1) . Its eigenvalues are the Matsubara frequencies $\omega_n = \gamma_1 \frac{2\pi n}{L_0}$, $n \in \mathbb{Z}$. Assuming that the Hamiltonian \tilde{H} has a translationally invariant vacuum and a mass gap, the right-hand side of Eq. (4.9) becomes insensitive to the phase in the limit $L_1 \rightarrow \infty$ at fixed ξ_1 (with exponentially small corrections, see below). This in turn implies that the free energy densities associated with V_{sbc} and $\text{diag}(L_1 \gamma_1, L_0 / \gamma_1, L_2, L_3)$ are equal. Thanks to the invariance of the infinite-volume theory under three-dimensional rotations, this result extends to a generic imaginary velocity $\boldsymbol{\xi}$. In the thermodynamic limit the net effect of the generic shift $\boldsymbol{\xi}$ is thus to lower the temperature from $1/L_0$ to $1/\beta = 1/(L_0 \sqrt{1 + \boldsymbol{\xi}^2})$, i.e. we have proved Eq. (2.5). As

anticipated in section 2, when the primitive cell dimensions L_k are all asymptotically large the system is characterized by a single ‘short’ periodic direction of length $\beta = L_0\sqrt{1+\xi^2}$ which is interpreted as being its inverse temperature. Its orientation is unusual in that it is not aligned along the time-direction, but due to its $\text{SO}(4)$ symmetry this is irrelevant.

In a finite-volume the length of the box dimensions are further sources of $\text{SO}(4)$ soft breakings, and the above analysis is significantly more involved. To go straight to the point, let us assume again that only $\xi_1 \neq 0$. The Euclidean finite-volume counterpart of the textbook relations (2.1) read

$$\begin{aligned}\langle T_{00} \rangle_{V_{\text{sbc}}} &= \gamma_1^2 \left(\langle T_{00} \rangle_{RV_{\text{sbc}}} + \xi_1^2 \langle T_{11} \rangle_{RV_{\text{sbc}}} \right) - 2\xi_1 \gamma_1^2 \langle T_{01} \rangle_{RV_{\text{sbc}}} , \\ \langle T_{01} \rangle_{V_{\text{sbc}}} &= \gamma_1^2 \left(\langle T_{00} \rangle_{RV_{\text{sbc}}} - \langle T_{11} \rangle_{RV_{\text{sbc}}} \right) \xi_1 + \gamma_1^2 (1 - \xi_1^2) \langle T_{01} \rangle_{RV_{\text{sbc}}} ,\end{aligned}\quad (4.10)$$

where in this case

$$RV_{\text{sbc}} \Big|_{\xi_2=\xi_3=0} = \begin{pmatrix} L_0/\gamma_1 & L_1\gamma_1\xi_1 & 0 & 0 \\ 0 & L_1\gamma_1 & 0 & 0 \\ 0 & 0 & L_2 & 0 \\ 0 & 0 & 0 & L_3 \end{pmatrix} . \quad (4.11)$$

In general the term on the r.h.s $\langle T_{01} \rangle_{RV_{\text{sbc}}}$ does not vanish in finite volume, while it does in the thermodynamic limit where Eqs. (2.1) are reproduced. Thus if we consider a thermal system satisfying ordinary spatial periodic boundary conditions ‘moving’ at imaginary velocity ξ , an attempt to ‘boost’ it back to the rest frame modifies its spatial boundary conditions in such a way that the momentum density does not vanish. This effect becomes irrelevant when the spatial correlation length is finite and the volume becomes large (see below). However, a remarkable property of periodic boundary conditions is that there are discrete values of the (imaginary) velocity for which the system at rest still obeys ordinary spatial periodic boundary conditions, and the textbook relations in Eqs. (2.1) hold. The term $\langle T_{01} \rangle_{RV_{\text{sbc}}}$ does vanish *in finite volume* when the parameters of the system satisfy

$$\frac{L_1\gamma_1^2\xi_1}{L_0} = q \in \mathbb{Z} . \quad (4.12)$$

Indeed Eq. (4.12) implies that $RV_{\text{sbc}}|_{\xi_2=\xi_3=0} \sim \text{diag}(L_0/\gamma_1, L_1\gamma_1, L_2, L_3)$ by an $\text{SL}(4, \mathbb{Z})$ transformation, see Eq. (3.4).

4.1 Finite-size effects

It is interesting to ask about the magnitude of finite-size corrections to Eq. (2.5). For a generic shift the effect of the finite value of L_1 in the free energy $f(V_1)$ can be quantified as

$$f(V_1) = \frac{1}{L_0 L_1 L_2 L_3} \left[L_1 \gamma_1 E_{\text{vac}}(\bar{V}_1) - \ln \left(1 + \nu \sum_{\text{1-particle states}} e^{-L_1 \gamma_1 (E + i \xi_1 p_1)} \right) \right] + \dots \quad (4.13)$$

where \bar{V}_1 is the $(0,0)$ minor of the matrix V_1 which describes the space on which the eigenstates of the Hamiltonian \tilde{H} are defined. The vacuum energy $E_{\text{vac}}(\bar{V}_1)$ on the space

\bar{V}_1 corresponds to the free energy of the system in the limit $L_1 \rightarrow \infty$. As indicated in Eq. (4.13), the leading correction

$$\mathcal{I}_1 = -\frac{\nu}{L_0 L_1 L_2 L_3} \sum_{\text{1-particle states}} e^{-L_1 \gamma_1 (E + i \xi_1 p_1)} \quad (4.14)$$

comes from one-particle states, where the factor ν stands for the multiplicity of the lightest screening state of mass M . The allowed momenta in the periodic box described by \bar{V}_1 are given by

$$\mathbf{p} = \begin{pmatrix} \frac{2\pi\gamma_1 n_1}{L_0} - \gamma_1 \xi_2 p_2 - \gamma_1 \xi_3 p_3 \\ p_2 \\ p_3 \end{pmatrix}, \quad p_2 = 2\pi \frac{n_2}{L_2}, \quad p_3 = 2\pi \frac{n_3}{L_3}, \quad \mathbf{n} \in \mathbb{Z}^3. \quad (4.15)$$

In the following we assume that a momentum of order $1/L_0$ always costs a substantial gap in energy, and therefore set $n_1 = 0$. Then \mathbf{p} is orthogonal to the short periodic direction $\mathbf{u}^\top \equiv (L_0/\gamma_1, L_0\xi_2, L_0\xi_3)$. When the box lengths L_2 and L_3 are large, we expect the dispersion relation of the one-particle states in momenta orthogonal to \mathbf{u} to be the ordinary relativistic dispersion relation, due to the emerging $\text{SO}(3)$ rotation symmetry in the space orthogonal to \mathbf{u} . The leading contribution thus reads

$$\mathcal{I}_1 = \frac{-\nu}{L_0 L_1 L_2 L_3} \sum_{p_2, p_3} e^{-L_1 \gamma_1 (\sqrt{M^2 + p_2^2 + p_3^2 + \gamma_1^2 (p_2 \xi_2 + p_3 \xi_3)^2} - i \xi_1 \gamma_1 (p_2 \xi_2 + p_3 \xi_3))}. \quad (4.16)$$

Using the Poisson summation formula, diagonalizing the quadratic form under the square root and appropriately rescaling the momentum integration variables, we arrive at

$$\mathcal{I}_1 = \frac{-\gamma\nu}{L_0 L_1 \gamma_1} \sum_{m_2, m_3 \in \mathbb{Z}} \int_{\mathbb{R}^2} \frac{d^2 \mathbf{p}}{(2\pi)^2} e^{-L_1 \gamma_1 \sqrt{M^2 + \mathbf{p}^2} + i \mathbf{p} \cdot \mathbf{x}} \quad (4.17)$$

with

$$\mathbf{x}^\top = \left(\frac{\gamma}{\gamma_1} \frac{(\xi_2^2 + \xi_3^2) L_1 \gamma_1^2 \xi_1 - m_2 L_2 \xi_2 - m_3 L_3 \xi_3}{\sqrt{\xi_2^2 + \xi_3^2}}, \frac{m_2 L_2 \xi_3 - m_3 L_3 \xi_2}{\sqrt{\xi_2^2 + \xi_3^2}} \right). \quad (4.18)$$

Using the observation that

$$\int \frac{d^2 \mathbf{p}}{(2\pi)^2} e^{-|x_1| \sqrt{M^2 + \mathbf{p}^2} + i \mathbf{p} \cdot \mathbf{x}} = -2 \frac{|x_1|}{r} \partial_r \Delta^3(r, M^2), \quad r = (x_1^2 + \mathbf{x}^2)^{1/2}, \quad (4.19)$$

where $\Delta^3(r, M^2)$ is the propagator of a free massive scalar particle on \mathbb{R}^3 , we finally obtain

$$\mathcal{I}_1 = \frac{\gamma\nu}{2\pi L_0} \sum_{m_2, m_3 \in \mathbb{Z}} \frac{1}{r} \frac{d}{dr} \left[\frac{e^{-Mr}}{r} \right]_{r=\sqrt{(Q\boldsymbol{\mu}, Q\boldsymbol{\mu})}}, \quad (4.20)$$

where $\boldsymbol{\mu} = (L_1, m_2 L_2, m_3 L_3)$, and $Q_{ij} = (\delta_{ij} + (\gamma - 1) \xi_i \xi_j / \boldsymbol{\xi}^2)$ defines a positive norm which takes into account the Euclidean version of relativistic length contraction in direction $\boldsymbol{\xi}$. The leading contribution to \mathcal{I}_1 is thus given by the value of (m_2, m_3) that minimizes the

norm of vector \mathbf{x} in Eq. (4.18), i.e.⁹ $m_2 = m_3 = 0$. The leading finite-volume effect associated with L_1 is thus

$$\mathcal{I}_1 = -\frac{\nu}{2\pi L_0 L_1^3} \frac{\gamma_{23}^3}{\gamma^2} \left[1 + mL_1 \frac{\gamma}{\gamma_{23}} \right] e^{-ML_1 \gamma / \gamma_{23}} . \quad (4.21)$$

To obtain the finite volume corrections to $E_{\text{vac}}(\bar{V}_1)$ due to the finiteness of the other spatial directions we can proceed iteratively as follows. A helpful observation is that in the limit $L_1 \rightarrow \infty$, the shift $-L_1 \gamma_1 \xi_1$ in V_1 can be ignored if the ground state is translationally invariant. We thus obtain

$$\gamma_1 E_{\text{vac}}(\bar{V}_1) = -\lim_{L_1 \rightarrow \infty} \frac{1}{L_1} \ln Z(V'_{\text{sbc}}), \quad (4.22)$$

where V'_{sbc} is obtained from V_{sbc} by making the two-step substitutions: first treat γ_1 as independent of ξ_1 and set

$$L_0 \rightarrow L_0 / \gamma_1, \quad L_1 \rightarrow L_1 \gamma_1, \quad \xi_1 \rightarrow 0, \quad \xi_2 \rightarrow \gamma_1 \xi_2, \quad \xi_3 \rightarrow \gamma_1 \xi_3, \quad (4.23)$$

and then assign to γ_1 its value in Eq. (4.6). The partition function in Eq. (4.22) can now be interpreted in terms of states living on slices of constant coordinate x_2 . The associated leading finite-size corrections are then given by \mathcal{I}_2 which, as expected, matches what one would obtain by cyclically permuting the three directions in expression (4.21). In summary, the leading finite-size contributions to the free energy are

$$f(V_{\text{sbc}}) - f(L_0 \sqrt{1 + \xi^2}) = \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3 + \dots \quad (4.24)$$

and the larger contribution(s) among those on the r.h.s. depends on the particular geometry of the shifted boundary conditions. As a test of this result, we perform an independent calculation for a free-boson theory in appendix C. It should be noted that, since the leading correction arises from one-particle states, the leading finite-size effects are predicted exactly by a free-boson theory if one sets its mass to M . The procedure followed in this section and the formula (4.24) generalize to shifted boundary conditions those in Ref. [9]. Also in this case the leading finite-volume corrections are fully determined once the mass M and the multiplicity ν of the lightest screening multiplet are known.

4.2 Ward identities for total energy and momentum

The equality $Z(V_{\text{sbc}}) = Z(V_k)$, where V_k is defined analogously to V_1 for the k -direction, can be used to generate WIs for correlators of the energy and momentum fields in a quasi-automated fashion. It suffices to take derivatives with respect to the parameters of the primitive vectors. If we derive once with respect to ξ_k , the first WI is given by

$$\langle T_{0k} \rangle_{V_{\text{sbc}}} + \frac{1 + \xi_k^2}{1 - \xi_k^2} \langle T_{0k} \rangle_{V_k} = \frac{\xi_k}{1 - \xi_k^2} \{ \langle T_{00} \rangle_{V_{\text{sbc}}} - \langle T_{kk} \rangle_{V_{\text{sbc}}} \} . \quad (4.25)$$

⁹If $L_1 \gg L_2, L_3$, several values of m_2 and m_3 make comparable contributions, and the original representation in terms of a sum over discrete momenta is more useful. However, in that case the finite-volume effects associated with the other directions will be the dominant ones anyhow.

The second term on the l.h.s proportional to $\langle T_{0k} \rangle_{V_k}$ vanishes in the limit $L_k \rightarrow \infty$, and as expected it vanishes also at finite L_k if the condition analogous to Eq. (4.12) is satisfied, i.e. $\frac{L_k \gamma_k^2 \xi_k}{L_0} = q \in \mathbb{Z}$. By differentiating twice with respect to ξ_k and by setting $\xi_k = 0$ we obtain

$$L_0 \langle \bar{T}_{0k} T_{0k} \rangle_{V_{\text{sbc},c}} - L_k \langle \tilde{T}_{0k} T_{0k} \rangle_{V_{\text{sbc},c}} = \langle T_{00} \rangle_{V_{\text{sbc}}} - \langle T_{kk} \rangle_{V_{\text{sbc}}}, \quad (4.26)$$

where all insertions in the same correlator are at a physical distance from each other and

$$\tilde{T}_{\mu\nu}(w_k) = \int \left[\prod_{\rho \neq k} dw_\rho \right] T_{\mu\nu}(w). \quad (4.27)$$

Analogously the fourth derivative leads to

$$\begin{aligned} L_0^3 \langle \bar{T}_{0k} \bar{T}_{0k} \bar{T}_{0k} T_{0k} \rangle_{V_{\text{sbc},c}} - L_k^3 \langle \tilde{T}_{0k} \tilde{T}_{0k} \tilde{T}_{0k} T_{0k} \rangle_{V_{\text{sbc},c}} &= 3 \left\{ \langle T_{00} \rangle_{V_{\text{sbc}}} - \langle T_{kk} \rangle_{V_{\text{sbc}}} \right\} + \\ 3 \left\{ L_k \langle \tilde{T}_{kk} T_{kk} \rangle_{V_{\text{sbc},c}} - L_0 \langle \bar{T}_{00} T_{00} \rangle_{V_{\text{sbc},c}} \right\} &+ 6 \left\{ L_0^2 \langle \bar{T}_{0k} \bar{T}_{0k} T_{00} \rangle_{V_{\text{sbc},c}} - L_k^2 \langle \tilde{T}_{0k} \tilde{T}_{0k} T_{kk} \rangle_{V_{\text{sbc},c}} \right\} \end{aligned} \quad (4.28)$$

after some rearrangements of the various terms, having set $\xi_k = 0$ again and having inserted all fields at a physical distance. This derivation extends to a generic thermal-field theory results previously obtained in the scalar field theory, Eqs. (5.3) and (6.15) in Ref. [2]. Again, due to the breaking of Lorentz symmetry, Eqs. (4.26) and (4.28) differ from those in (2.12) by terms which vanish in the thermodynamic limit.

5. Applications on the lattice

The shifted boundary conditions discussed so far provide an interesting formulation to study thermal field theories on the lattice. There are many applications that can potentially benefit from them. In this section we sketch a few examples with the computation of thermodynamic potentials in mind.

5.1 Renormalization of the energy-momentum tensor

In the continuum, the charges associated with translational symmetries, i.e. the total energy and momentum fields, do not need any ultraviolet renormalization thanks to the Ward identities that they satisfy, for a recent discussion see Ref. [2] and references therein. On the lattice, however, translational invariance is broken down to a discrete group and the standard charge discretizations acquire finite ultraviolet renormalizations. The renormalization pattern of the energy-momentum tensor depends on the theory under consideration, since its field content determines what operators $T_{\mu\nu}$ can mix with. For definiteness the discussion below focuses on the $\text{SU}(N)$ Yang–Mills theory, but it applies to the scalar field theory as well.

The energy-momentum field $T_{\mu\nu}$ is a symmetric rank-two tensor. Its traceless part is an irreducible representation of the $\text{SO}(4)$ group. On the lattice, however, the diagonal and off-diagonal components of this multiplet belong to different irreducible representations of the hypercubic lattice symmetry group and therefore renormalize in a different way. In $\text{SU}(N)$ Yang–Mills theory, they both renormalize multiplicatively. The WIs (4.25)

and (4.26) provide two relations among the expectation values of the diagonal and off-diagonal components of the energy-momentum tensor. They can be enforced on the lattice to compute the overall renormalization constant Z_T of the multiplet, and the relative normalization z_T between the off-diagonal and the diagonal components [10, 11],

$$T_{01}^R = Z_T T_{01}, \quad T_{00}^R - T_{11}^R = Z_T z_T (T_{00} - T_{11}), \quad \text{etc.} \quad (5.1)$$

where the fields with a superscript ‘R’ are the renormalized ones. There are many ways to implement this strategy in practice. A possible choice is to require a primitive matrix

$$V_T = \begin{pmatrix} L_0 & 0 & 0 & 0 \\ \frac{L_0}{2} & \frac{5}{2}L_0 & 0 & 0 \\ 0 & 0 & L & 0 \\ 0 & 0 & 0 & L \end{pmatrix} \quad (5.2)$$

for which the condition (4.12) holds, and compute z_T as

$$z_T = \frac{3}{2} \frac{\langle T_{01} \rangle_{V_T}}{\langle T_{00} \rangle_{V_T} - \langle T_{11} \rangle_{V_T}}, \quad (5.3)$$

while Z_T can be determined from $(x_0 \neq y_0, x_2 \neq y_2)$

$$\frac{Z_T}{z_T} = \frac{\langle T_{00} \rangle_{V_T} - \langle T_{22} \rangle_{V_T}}{L_0 \langle \bar{T}_{02}(x_0) T_{02}(y) \rangle_{V_T, c} - L \langle \tilde{T}_{02}(x_2) T_{02}(y) \rangle_{V_T, c}}. \quad (5.4)$$

Being fixed by WIs, the finite renormalization constants Z_T and z_T depend on the bare coupling constant only. Up to discretization effects, they are independent of the kinematics used to impose them, e.g. the volume, the temperature, the shift parameter, x_0 etc. Ultimately which WIs and/or kinematics yield the most accurate results must be investigated numerically.

5.2 Calculation of the entropy and specific heat

Once the relevant renormalization constants are determined, the entropy density can be computed from the expectation value of T_{0k} on a lattice with shifted boundary conditions,

$$s = - \frac{Z_T L_0 (1 + \xi^2)^{3/2}}{\xi_k} \langle T_{0k} \rangle_{\xi}, \quad \xi_k \neq 0, \quad (5.5)$$

by performing simulations at a single inverse temperature value $\beta = L_0 \sqrt{1 + \xi^2}$, and at a volume large enough for finite-size effects to be negligible. The latter are exponentially small in (ML) , where M is the lightest screening mass of the theory. To properly assess discretization effects, a set of full-fledged simulations needs to be performed at several lattice spacings. A rough idea on their magnitude, however, can be obtained in the non-interacting limit of the theory. For the $SU(N)$ Yang–Mills theory discretized with the Wilson action and for the ‘clover’ form of the lattice field strength tensor [12], discretization effects turn out to be rather small, see Fig. 1 for the choice corresponding to $\xi = (1, 0, 0)$. The details of the calculation are given in appendix D. Once the entropy has been computed

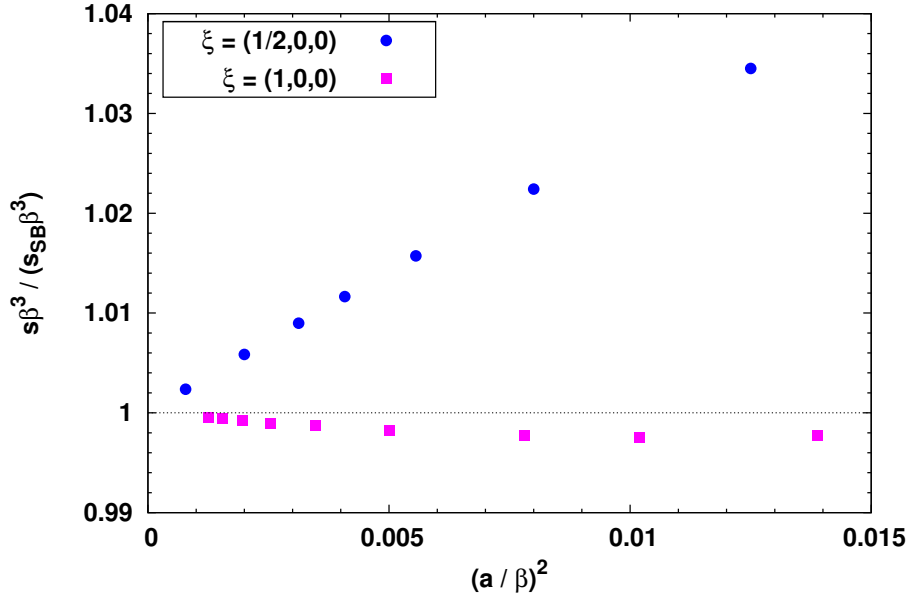


Figure 1: Entropy density at finite lattice spacing for the $SU(N)$ Yang-Mills theory in the non-interacting limit calculated via Eq. (5.5) and normalized to its continuum value $s_{\text{SB}}\beta^3 = \frac{4\pi^2(N^2-1)}{45}$. The discretization used is the Wilson action and the ‘clover’ form of the lattice field strength tensor, see appendix D. The inverse temperature is $\beta = L_0\sqrt{1+\xi^2}$, and a is the lattice spacing.

at various values of β , the pressure can be computed by integrating s in the temperature. The ambiguity left due to the integration constant is consistent with the fact that p is defined up to an arbitrary additive renormalization constant.

The entropy density could also be computed directly from Eq. (2.18) without the need for fixing the multiplicative renormalization constant. This would require, however, the computation of the two-point correlation functions in a large volume. The latter can also be used to access the specific heat of the system. From Eqs. (2.18) and (2.19), by choosing all L_k and all ξ_k equal, for instance, the speed of sound c_s is given by

$$\frac{1}{c_s^2} = \frac{c_v}{s} = \frac{3}{\xi^2} \frac{\langle \bar{T}_{01} T_{02} \rangle_{\xi,c} + \xi^2 \langle \bar{T}_{01} T_{01} \rangle_{\xi,c}}{\langle \bar{T}_{01} T_{02} \rangle_{\xi,c} - \langle \bar{T}_{01} T_{01} \rangle_{\xi,c}}, \quad (5.6)$$

where as usual in each correlator all fields are inserted at physical distance. Note that without shifted boundary conditions, the specific heat would require the computation of a four-point function of \bar{T}_{0k} [1, 2]. Note also that all the computational strategies sketched in this section use correlation functions of local operators that require at most an overall renormalization constant. The latter can be fixed by WIs in finite volume as described in the previous sub-section, and no ultraviolet power-divergent subtractions are needed.

5.3 The integral method at fixed shift

Calculations of thermodynamic quantities in lattice gauge theories (see [13] for a recent review) usually focus on obtaining the pressure p . In the thermodynamic limit and for a

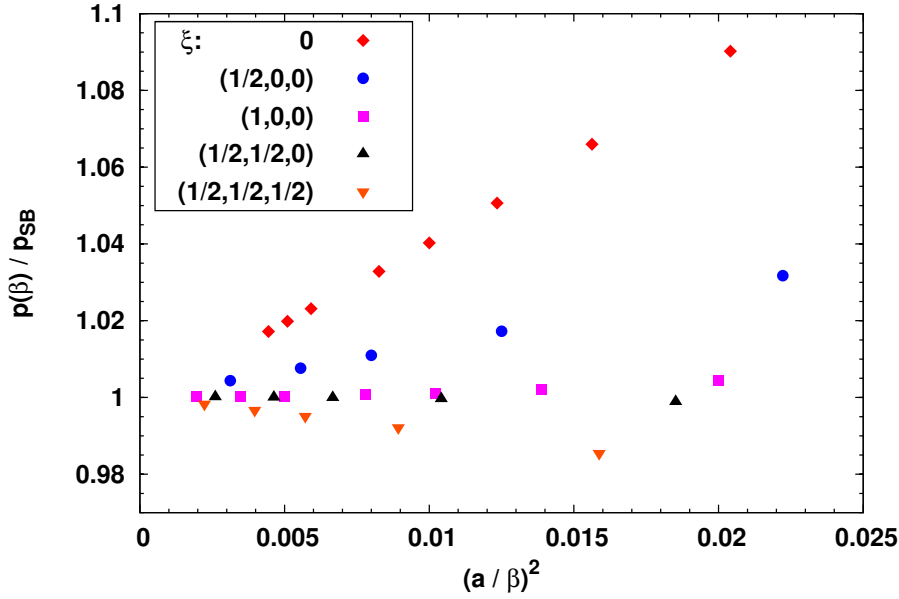


Figure 2: Pressure at finite lattice spacing for the $SU(N)$ Yang–Mills theory in the non-interacting limit. The discretization used is the Wilson action and the ‘clover’ form of the lattice field strength tensor. The inverse temperature is given by $\beta = L_0 \sqrt{1 + \xi^2}$, and a is the lattice spacing.

homogeneous system, the pressure is equal to minus the free energy, $p = -f$, and all other thermodynamic potentials can in principle be derived from it by taking derivatives with respect to the temperature. In the original integral method proposal [14], the pressure p is computed by carrying out a line integral of the gradient of the logarithm of the partition function with respect to the bare parameters. The integrand is expressed as an expectation value of derivatives of the action with respect to the bare parameters $\alpha = (\alpha_1, \dots, \alpha_n)$. Starting the integration from a point where by convention the free energy vanishes, one obtains

$$p(L_0) = -\frac{1}{L_0 L^3} \int_{\alpha_1}^{\alpha_2} d\alpha \cdot \langle \nabla_{\alpha} S \rangle_{\alpha} , \quad (5.7)$$

where S is the lattice action and $\langle \dots \rangle_{\alpha}$ is an expectation value taken at the bare parameter set α . The integral is done by keeping fixed L_0/a , and the temperature is changed by varying the lattice spacing. The latter is achieved by varying the bare coupling, but in doing so the other couplings (if any) must be adjusted if one wants to remain on a line of constant physics. Moreover a subtraction of the vacuum contribution must be made in evaluating the path-integral expectation value of $\frac{\partial S}{\partial \alpha_k}$, which is usually done at a temperature different from the target temperature, or even at zero temperature [14, 15]. Thanks to the integral method, many results have been obtained on the lattice for thermal gauge theories [13]. Due to the vacuum subtraction and to the integral on the bare parameters at constant physics, it remains difficult, however, to reach large temperatures or to apply this method to regularizations where the tuning of the bare parameters is technically demanding.

The integral method can also be applied in the presence of shifted boundary conditions. For a given inverse temperature $\beta = L_0 \sqrt{1 + \xi^2}$, the continuum limit $\beta/a \rightarrow \infty$ of $p\beta^4$

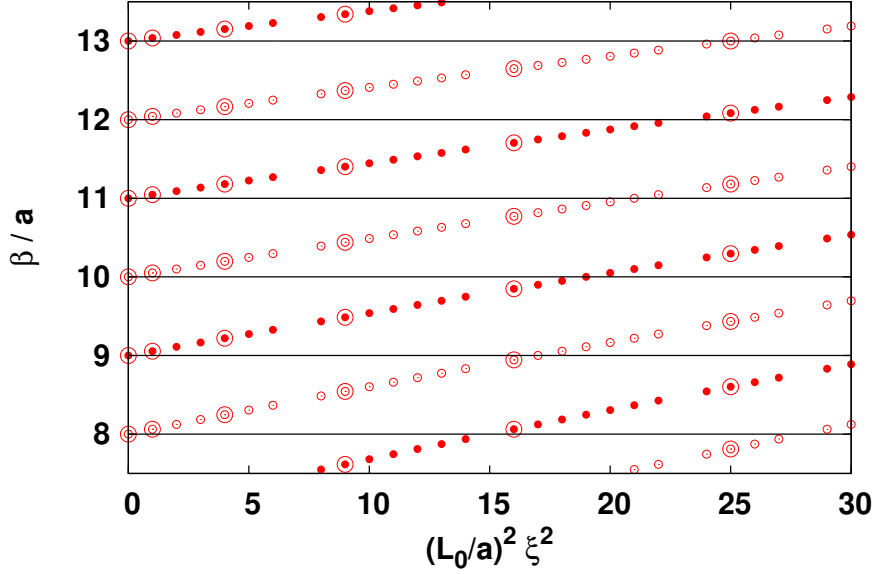


Figure 3: Inverse temperature values that become accessible with the use of shifted boundary conditions at a fixed lattice spacing a and for different values of L_0/a . The inverse temperatures accessible with a shift in a single direction, $\xi = (\xi_1, 0, 0)$, are marked by a double circle.

can be taken at fixed ξ . This means that the angles among the lattice axes and the torus directions are kept fixed. The discretization effects on $p\beta^4$ in the non-interacting limit of the $SU(N)$ Yang–Mills theory are displayed in Fig. 2. The plot shows that, in the free theory, they can be drastically reduced by using shifted boundary conditions. It remains to be seen whether this fact persists in the interacting theory.

5.4 Temperature scan at fixed lattice spacing

The possibility of varying the temperature by changing either L_0/a or ξ allows for a fine scan of the temperature axis at fixed lattice spacing. This is illustrated in Fig. 3, where it is also compared with the standard procedure of varying L_0/a only. This fact may turn out to be useful in all those cases where the temperature needs to be changed in small steps, e.g. study of phase transitions etc.

The ‘T-integral’ method [16] is an approach for computing thermodynamic quantities related to the integral method which is however formulated directly in the continuum. Here the pressure is computed as the integral

$$p(\beta_2) = \frac{\beta_1^4}{\beta_2^4} p(\beta_1) - \frac{1}{\beta_2^4} \int_{\beta_1}^{\beta_2} d\beta \beta^3 [e(\beta) - 3p(\beta)] , \quad (5.8)$$

with the integrand computed by Monte Carlo simulations, and the inverse temperature β is varied by changing L_0/a while keeping the bare parameters (bare coupling, quark masses, ...) of the theory fixed. This method has a number of advantages over the method based on Eq. (5.7). The subtraction of the vacuum contribution only requires a single zero-temperature simulation, and no tuning of bare parameters is required to perform a scan in

temperature. A significant drawback however is that for a given, realistic ($L_0/a = 8 \dots 20$) lattice spacing the temperature can only be varied in rather coarse steps. The shifted boundary conditions provide a way to almost completely eliminate this drawback. Since the integrand is a Lorentz-scalar, its expectation value in the presence of the shifted boundary condition is equal, up to discretization effects, to its expectation value in the unshifted ensemble at inverse temperature $\beta = L_0 \sqrt{1 + \xi^2}$. The integrand can thus be scanned in much finer steps, and the integral can be computed as

$$p(L_0) = (1 + \xi^2)^2 p(L_0 \sqrt{1 + \xi^2}) + \frac{1}{2} \int_0^{\xi^2} dy (1 + y) \left[e(L_0 \sqrt{1 + \xi'^2}) - 3p(L_0 \sqrt{1 + \xi'^2}) \right]_{\xi'^2=y} \quad (5.9)$$

The shifted boundary conditions and the associated WIs also suggest a different implementation of the method. Thanks to Eq. (5.5), and by remembering that $\beta^2 \frac{\partial}{\partial \beta} p = -s$, the pressure difference at two temperatures and at a given lattice spacing can be computed for instance as

$$p(L_0 \sqrt{2}) = p\left(L_0 \sqrt{2 + \xi_\perp^2}\right) - \frac{Z_T}{2} \int_0^{\xi_\perp^2} dy \langle T_{0k} \rangle_{\xi'} \Big|_{\xi_\perp'^2=y} \quad (5.10)$$

where $\xi'_k = 1$ and ξ'_\perp stands for the two components orthogonal to the k -direction.

6. Conclusions

Lorentz invariance implies a great degree of redundancy in defining a relativistic thermal theory in the Euclidean path-integral formalism. In the thermodynamic limit, the orientation of the compact periodic direction with respect to the coordinate axes can be chosen at will and only its length is physically relevant. This redundancy in the description implies that the total energy and momentum distributions in the canonical ensemble are related.

For a finite-size system, the lengths of the box dimensions break this invariance. The orientation of the Matsubara cycle relative to the spatial directions does have effects which, however, are exponentially suppressed. In the limit of large spatial volume the latter are calculable in terms of the mass and multiplicity of the lightest screening state(s) of the theory. Being a soft breaking, the correlation functions of the traceless part of the energy-momentum tensor still satisfy exact Ward Identities.

When the theory is regularized in the ultraviolet on a hypercubic lattice, the latter singles out a particular reference frame. The overall orientation of the periodic cycles of the finite-volume, finite-temperature system with respect to this preferred coordinate system affects renormalized observables at the level of lattice artifacts. As the cutoff is removed, the artifacts are suppressed by a power of the lattice spacing.

The shifted boundary condition introduced in [1, 2] constitute a particularly interesting instance of the generalized boundary conditions described in section 3. In the language of the canonical formalism, the energy eigenstates acquire a phase proportional to their momentum. This different but equivalent point of view implies that thermodynamic potentials can be directly inferred from the response of the partition function to the shift in the boundary conditions [1, 2], a response which is also encoded in the expectation value and in the correlators of the off-diagonal components of the energy-momentum tensor.

The flexibility in the lattice formulation added by the introduction of a triplet ξ of (renormalized) parameters specifying the temporal boundary condition has interesting applications. It suggests new and simpler ways to compute thermodynamic potentials, and the Ward identities mentioned above can be enforced in a small volume to determine the renormalization constants of the energy-momentum tensor components. The temperature can be changed either by varying L_0 in multiples of the lattice spacing or via the shift parameters ξ . This results in a much finer scan of its value at fixed bare parameters, a feature that may prove particularly useful in investigations of phase transitions (see for instance [17]).

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A. Derivation of Eq. (2.10)

The Eq. (2.9), which expresses a linear relation between the c_1, \dots, c_n and the n first derivatives of the free energy density, is readily inverted

$$L_0^{n+1} \frac{\partial^n f}{\partial L_0^n} = (-1)^{n+1} n! \sum_{k=1}^n \frac{1}{k!} L_0^k c_k, \quad n = 1, 2, \dots \quad (\text{A.1})$$

On the other hand, after some algebra, it is possible to show that

$$\left(\frac{1}{L_0} \frac{\partial}{\partial L_0} \right)^n f = \frac{1}{L_0^{2n}} \sum_{k=1}^n \frac{(-1)^{n-k}}{2^{n-k}} \frac{(2n-k-1)!}{(k-1)!(n-k)!} L_0^k \frac{\partial^k f}{\partial L_0^k}, \quad n = 1, 2, \dots \quad (\text{A.2})$$

Using first Eq. (A.2) and then (A.1), the derivatives of the free energy in expression (2.7) can be replaced by the c_n . One then arrives at the desired relation between the cumulants of the momentum and the energy operator, Eq. (2.10).

B. Momentum-space analysis of GPBCs

Since translational invariance is left unbroken by the boundary conditions, we can expand the fields in Fourier modes. The set of momenta compatible with the boundary conditions is¹⁰

$$\Gamma_V = \left\{ p \in \mathbb{R}^d \mid p_\mu = 2\pi(V^{-1})_{\nu\mu} n_\nu, \ n_\nu \in \mathbb{Z} \right\} \quad (\text{B.1})$$

¹⁰In crystallographic terminology this is the *reciprocal lattice*.

and the plane wave expansion reads

$$\phi_\sigma(x) = \sum_{p \in \Gamma_V} \tilde{\phi}_\sigma(p) e^{ip \cdot x} = \phi_\sigma(x + Vm), \quad (Vm)_\mu = V_{\mu\nu} m_\nu, \quad m_\nu \in \mathbb{Z}. \quad (\text{B.2})$$

Clearly, we have the property

$$\Gamma_V = \Gamma_{VM}, \quad M \in \text{SL}(d, \mathbb{Z}). \quad (\text{B.3})$$

It is instructive to see how the equivalence (3.5) shows up in momentum space. First, consider a term S_n^∞ in the action of the infinite-volume theory

$$S_n^\infty([\phi]) = \int \left(\prod_{i=1}^n \frac{d^d p^i}{(2\pi)^d} \right) c_n^{\sigma_1 \dots \sigma_n}(p^1, \dots, p^n) \tilde{\phi}_{\sigma_1}(p^1) \dots \tilde{\phi}_{\sigma_n}(p^n) (2\pi)^d \delta^{(d)}\left(\sum_{i=1}^n p^i\right), \quad (\text{B.4})$$

where as usual the delta function enforces momentum conservation in all d directions. Since the fields are irreducible representations, Lorentz symmetry is encoded in the property

$$\begin{aligned} c_n^{\sigma_1 \dots \sigma_n}(p^1, \dots, p^n) \tilde{\phi}_{\sigma_1}^\Lambda(p^1) \dots \tilde{\phi}_{\sigma_n}^\Lambda(p^n) \\ = c_n^{\sigma_1 \dots \sigma_n}(\Lambda^{-1}p^1, \dots, \Lambda^{-1}p^n) \tilde{\phi}_{\sigma_1}(\Lambda^{-1}p^1) \dots \tilde{\phi}_{\sigma_n}(\Lambda^{-1}p^n), \end{aligned} \quad (\text{B.5})$$

i.e. the action density at momenta (p_1, \dots, p_n) of the rotated field

$$\tilde{\phi}_\sigma^\Lambda(p) \equiv U(\Lambda)_{\sigma\sigma'} \tilde{\phi}_{\sigma'}(\Lambda^{-1}p) \quad (\text{B.6})$$

is the same as the action density of the original field at momenta $(\Lambda^{-1}p_1, \dots, \Lambda^{-1}p_n)$. This property guarantees in particular that the infinite-volume action of a rotated field is equal to the action of the original field.

In the finite-volume theory, the same form of the action holds, but the integral over momenta is replaced by a sum over the set Γ_V of momenta compatible with the periodicity of the field. We can write this contribution to the action as

$$S_n(V; [\phi]) = \frac{1}{V_d^{n-1}} \sum_{p^i \in \Gamma_V} c_n^{\sigma_1 \dots \sigma_n}(p^1, \dots, p^n) \delta_{\sum_{i=1}^n p^i} \tilde{\phi}_{\sigma_1}(p^1) \dots \tilde{\phi}_{\sigma_n}(p^n), \quad (\text{B.7})$$

where V_d is the volume of the primitive cell. Clearly Eq. (B.3) implies that the action of the two systems parameterized by V and VM are equal *for the same field*,

$$S_n(V; [\phi]) = S_n(VM; [\phi]). \quad (\text{B.8})$$

Second, we can also write

$$S_n(V; [\phi]) = \frac{1}{V_d^{n-1}} \sum_{p^i \in \Gamma_{\Lambda V}} c_n^{\sigma_1 \dots \sigma_n}(\Lambda^{-1}p^1, \dots, \Lambda^{-1}p^n) \delta_{\sum_{i=1}^n p^i} \tilde{\phi}_{\sigma_1}(\Lambda^{-1}p^1) \dots \tilde{\phi}_{\sigma_n}(\Lambda^{-1}p^n), \quad (\text{B.9})$$

and by using Eq. (B.5) one finds

$$S_n(V; [\phi]) = S_n(\Lambda V; [\phi^\Lambda]). \quad (\text{B.10})$$

One immediate implication of Eq. (B.8) and (B.10) is that the partition functions of the same field theory with equivalent sets of boundary conditions V and $W = \Lambda V M$ are equal

$$V \sim W \quad \Rightarrow \quad Z(V) = Z(W). \quad (\text{B.11})$$

B.1 An alternative representation of a field theory with GPBCs

We return briefly to the plane wave expansion of the field, Eq. (B.2), to mention an alternative representation of a field theory with GPBCs. The rotation matrix Λ can always be chosen such that V is triangular. By denoting $V_{\mu\mu} = L_\mu$, we can write $V = (R^\top)^{-1}D$, where R is triangular and all its diagonal elements are unity, and $D = \text{diag}(L_0, \dots, L_{d-1})$. Consider then the field transformation

$$\hat{\phi}_\sigma(x) \equiv \phi_\sigma(R^{-1\top}x) . \quad (\text{B.12})$$

By expanding $\hat{\phi}(x)$ in Fourier modes

$$\hat{\phi}_\sigma(x) = \sum_{p=2\pi D^{-1}n} \tilde{\phi}_\sigma(p) e^{ip \cdot x}, \quad (\text{B.13})$$

in momentum space Eq. (B.12) becomes

$$\tilde{\phi}_\sigma(p) = \tilde{\phi}_\sigma(Rp) . \quad (\text{B.14})$$

From both Eq. (B.12) and Eq. (B.13), it is clear that $\hat{\phi}$ fulfills ordinary periodic boundary conditions on a primitive cell with d orthogonal sides of lengths (L_0, \dots, L_{d-1}) . The effect of the non-orthogonality of the original primitive vectors is absorbed into the action for $\hat{\phi}$,

$$\hat{S}_n(V; [\hat{\phi}]) \equiv S_n(V; [\phi]) = \frac{1}{V_d^{n-1}} \sum_{p^i \in \Gamma_D} c_n^{\sigma_1 \dots \sigma_n}(Rp^1, \dots, Rp^n) \delta_{\sum_{i=1}^n p^i} \tilde{\phi}_{\sigma_1}(p^1) \dots \tilde{\phi}_{\sigma_n}(p^n). \quad (\text{B.15})$$

The kinetic term of a scalar field theory, for instance,

$$c_2(Rp^1, Rp^2) = -\frac{1}{2} p^{1\top} (R^\top R) p^2$$

is a positive-definite quadratic form in this formulation.

C. Free energy of a non-interacting bosonic theory with shifted boundaries

In this appendix we compute the free-energy of a non-interacting bosonic field theory in a finite volume. This serve to check Eq. (4.24) in the free theory explicitly, and it also shows that the latter predicts correctly the leading finite-size effects for a generic thermal theory if the mass and the multiplicity are fixed to those of the lightest screening state(s).

For a generic set of GPBCs, the $\text{SO}(4)$ symmetry allows one to cast the primitive matrix \mathcal{V} in the form

$$\mathcal{V} = \begin{pmatrix} L_0 & 0 & 0 & 0 \\ z_1 & & & \\ z_3 & \bar{\mathcal{V}} & & \\ z_3 & & & \end{pmatrix}, \quad (\text{C.1})$$

see Eq. (3.3). The matrix $\bar{\mathcal{V}}$ specifies the spatial periodic directions of the system, and the associated three-dimensional reciprocal lattice can be extracted from Eq. (B.1). It is easy

to prove that

$$\begin{aligned} f(\mathcal{V}) - \lim_{L_0 \rightarrow \infty} f(\mathcal{V}) &= \frac{1}{L_0 \det \bar{\mathcal{V}}} \sum_{\mathbf{p}} \log(1 - e^{-L_0 \omega_{\mathbf{p}} + i\mathbf{p} \cdot \mathbf{z}}) \\ &= \frac{2}{L_0 \det \bar{\mathcal{V}}} \frac{\partial}{\partial L_0} \sum_{n \geq 1} \frac{1}{n^2} \sum_{\mathbf{p}} \frac{e^{n(-L_0 \omega_{\mathbf{p}} + i\mathbf{p} \cdot \mathbf{z})}}{2\omega_{\mathbf{p}}}, \end{aligned} \quad (\text{C.2})$$

where $\omega_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + M^2}$. Thanks to the Poisson summation formula

$$\frac{1}{\det \bar{\mathcal{V}}} \sum_{\mathbf{p}} \frac{e^{n(-L_0 \omega_{\mathbf{p}} + i\mathbf{p} \cdot \mathbf{z})}}{2\omega_{\mathbf{p}}} = \sum_{\mathbf{k} \in \mathbb{Z}^3} \Delta^4(r, M^2) \Big|_{r=\sqrt{n^2 L_0^2 + (n\mathbf{z} + \bar{\mathcal{V}}\mathbf{k})^2}}, \quad (\text{C.3})$$

where in d -dimensions

$$\Delta^d(|x|, M^2) \equiv \int \frac{d^d p}{(2\pi)^d} \frac{e^{ipx}}{p^2 + M^2}. \quad (\text{C.4})$$

We can thus write

$$f(\mathcal{V}) - \lim_{L_0 \rightarrow \infty} f(\mathcal{V}) = \sum_{k_0 \neq 0} \sum_{\mathbf{k}} \left[\frac{1}{r} \frac{\partial}{\partial r} \Delta^4(r, M^2) \right]_{r=|\mathcal{V}\mathbf{k}|}, \quad k^\top = (k_0, \mathbf{k}) \in \mathbb{Z}^4. \quad (\text{C.5})$$

By repeating the argument in all k -directions, i.e. by sending successively V_{kk} to infinity, we arrive at the master equation

$$f(\mathcal{V}) - f_\infty = \sum_{k \neq 0} \left[\frac{1}{r} \frac{\partial}{\partial r} \Delta^4(r, M^2) \right]_{r=|\mathcal{V}\mathbf{k}|}. \quad (\text{C.6})$$

where f_∞ is the free energy of the system on \mathbb{R}^4 , i.e. in infinite volume. Since Eq. (C.6) is expressed in terms of the norm of all the position vectors equivalent by periodicity to the origin, its form is invariant within an equivalence class of primitive matrices. It therefore holds for any $\mathcal{V} \in GL(4, \mathbb{R})$.

As an application of Eq. (C.6), we consider the case where \mathcal{V} is equal to V_{sbc} defined in Eq. (4.2), i.e.

$$f(V_{\text{sbc}}) - \lim_{L_1, L_2, L_3 \rightarrow \infty} f(V_{\text{sbc}}) = \mathcal{J} \equiv \sum_{n \in \mathbb{Z}} \sum_{\mathbf{m} \neq 0} \left[\frac{1}{r} \frac{\partial}{\partial r} \Delta^4(r, M^2) \right]_{r=\sqrt{n^2 L_0^2 + (nL_0 \boldsymbol{\xi} + \boldsymbol{\mu})^2}} \quad (\text{C.7})$$

where $\boldsymbol{\mu} = (m_1 L_1, m_2 L_2, m_3 L_3)$. Expression (C.7) involves 4d propagators, while Eq. (4.20) contains 3d propagators. Using again the Poisson formula, one obtains

$$\mathcal{J} = \sum_{m_0 \in \mathbb{Z}} \sum_{\mathbf{m} \neq 0} \int_{-\infty}^{\infty} d\eta e^{i2\pi m_0 \eta} \left[\frac{1}{r} \frac{\partial}{\partial r} \Delta^4(r, M^2) \right]_{r=\sqrt{\eta^2 L_0^2 + (\eta L_0 \boldsymbol{\xi} + \boldsymbol{\mu})^2}}, \quad (\text{C.8})$$

where the argument of the propagator can be rewritten as

$$r^2 = \eta^2 L_0^2 + (\eta L_0 \boldsymbol{\xi} + \boldsymbol{\mu})^2 = \frac{1}{\gamma^2} (\eta L_0 + \gamma^2 \boldsymbol{\xi} \cdot \boldsymbol{\mu})^2 + (Q\boldsymbol{\mu}, Q\boldsymbol{\mu}) \quad (\text{C.9})$$

with Q_{ij} being defined below Eq. (4.20). By setting $x_0 = (\eta L_0/\gamma + \gamma \boldsymbol{\xi} \cdot \boldsymbol{\mu})$, and by using the ‘dimensional reduction’ relation between the four- and three-dimensional propagators

$$\int_{-\infty}^{\infty} \frac{dx_0}{x_0} e^{-i\omega x_0} \frac{\partial}{\partial x_0} \Delta^4(|x|, M^2) = \left[\frac{1}{r} \frac{\partial}{\partial r} \Delta^3(r, \omega^2 + M^2) \right]_{r=|x|}, \quad (\text{C.10})$$

the following result emerges

$$\mathcal{J} = \frac{\gamma}{L_0} \sum_{m_0} \sum_{\boldsymbol{m} \neq 0} e^{-i2\pi m_0 \gamma^2 (\boldsymbol{\xi} \cdot \boldsymbol{\mu})/L_0} \left[\frac{1}{r} \frac{\partial}{\partial r} \Delta^3(r, M^2 + (2\pi m_0 \gamma/L_0)^2) \right]_{r=|Q\boldsymbol{\mu}|}. \quad (\text{C.11})$$

For large spatial box dimensions L_k , we can drop all terms but $m_0 = 0$ and obtain

$$\mathcal{J} = \frac{\gamma}{L_0} \sum_{\boldsymbol{\mu} \neq 0} \left[\frac{1}{r} \frac{\partial}{\partial r} \Delta^3(r, M^2) \right]_{r=|Q\boldsymbol{\mu}|} + \dots, \quad \Delta^3(r, M^2) = \frac{1}{4\pi r} e^{-Mr}. \quad (\text{C.12})$$

Taking into account that the relevant terms in $\boldsymbol{\mu}$ that give the leading correction in L_1 are now $\mu_1 = \pm L_1$, $\mu_2 = \mu_3 = 0$, we recover exactly Eq. (4.20) and therefore Eq. (4.24), if we set the mass and the multiplicity in the free-theory equal to those of the lightest screening state in the interacting theory.

D. Free bosonic theory on the lattice with shifted boundary conditions

On a finite-volume lattice specified by the primitive matrix V_{sbc} in Eq. (4.2), the bosonic propagator in position space reads¹¹

$$\Delta_L^4(x, M^2) = \frac{1}{L_0 L_1 L_2 L_3} \sum_{\ell=0}^{L_0-1} \sum_{\boldsymbol{p} \in BZ} \frac{e^{i(\frac{2\pi\ell}{L_0} - \boldsymbol{p} \cdot \boldsymbol{\xi})x_0 + i\boldsymbol{p} \cdot \boldsymbol{x}}}{4 \sin^2(\frac{\pi\ell}{L_0} - \frac{\boldsymbol{p} \cdot \boldsymbol{\xi}}{2}) + M^2 + 4 \sum_{k=1}^3 \sin^2(\frac{p_k}{2})}, \quad (\text{D.1})$$

where BZ stands for the Brillouin zone. We are thus interested in the finite sum

$$\Sigma(x_0) = \frac{1}{L_0} \sum_{\ell=0}^{L_0-1} \frac{e^{ix_0(2\pi\ell/L_0 - \phi)}}{\omega^2 + 4 \sin^2(\frac{\pi\ell}{L_0} - \frac{\phi}{2})}, \quad (\text{D.2})$$

and for each value of \boldsymbol{p} we will set

$$\phi = \boldsymbol{p} \cdot \boldsymbol{\xi}, \quad \omega^2 = M^2 + 4 \sum_{k=1}^3 \sin^2(\frac{p_k}{2}) \quad (\text{D.3})$$

at the end of the calculation. To this end we generalize a well known contour integral calculation, see for instance Ref. [18]. The first observation is that

$$\Sigma(x_0) = \frac{1}{L_0} \sum_{\ell=0}^{L_0-1} g(e^{i\pi\ell/L_0 - i\phi/2}, x_0), \quad g(z, x_0) = \frac{z^{2x_0}}{\omega^2 - (z - z^{-1})^2}, \quad (\text{D.4})$$

¹¹The lattice spacing is set to $a = 1$ in this appendix.

and using the fact that $g(z, x_0) = g(-z, x_0)$ we have

$$\Sigma(x_0) = \frac{1}{2L_0} \sum_{\ell=0}^{2L_0-1} g(e^{i\pi\ell/L_0-i\phi/2}, x_0) . \quad (\text{D.5})$$

The poles of $g(z, x_0)$ in the variable z are on the real axis at

$$\bar{z}_{1,\dots,4} = \pm \frac{\omega}{2} \pm \sqrt{\left(\frac{\omega}{2}\right)^2 + 1} . \quad (\text{D.6})$$

Consider the integral

$$I_{\text{all}} = \int_{\Gamma_{\text{all}}} \frac{dz}{z} \frac{g(z, x_0)}{e^{iL_0\phi} z^{2L_0} - 1} , \quad (\text{D.7})$$

where the contour Γ_{all} contains all the singularities of the integrand. The latter are all simple poles located at

$$\bar{z}_1, \bar{z}_2, \bar{z}_3, \bar{z}_4 ; \quad \hat{z}_\ell = e^{i\pi\ell/L_0-i\phi/2}, \quad \ell = 0, 1, \dots, (2L_0 - 1) . \quad (\text{D.8})$$

The integral I_{all} vanishes since the integrand falls off as $|z|^{-5}$ when $|z| \rightarrow \infty$. As a consequence the sum of all residues is null, and the sum of the residues at \bar{z}_i equals minus the sum of the residues at \hat{z}_ℓ . Since

$$e^{iL_0\phi} z^{2L_0} - 1 = (z_\phi - e^{i\pi\ell/L_0}) \left[z_\phi^{2L_0-1} + e^{i\pi\ell/L_0} z_\phi^{2L_0-2} + \dots + e^{i\pi\ell(2L_0-2)/L_0} z_\phi + e^{i\pi(2L_0-1)/L_0} \right] \quad (\text{D.9})$$

with $z_\phi \equiv ze^{i\phi/2}$, the residue of the integrand in Eq. (D.7) at \hat{z}_ℓ is

$$\frac{1}{2L_0} g(e^{i\pi\ell/L_0-i\phi/2}, x_0) . \quad (\text{D.10})$$

Comparing with Eq. (D.5) we have

$$\Sigma(x_0) = \frac{1}{2\pi i} \int_{\hat{\Gamma}} \frac{dz}{z} \frac{g(z, x_0)}{e^{iL_0\phi} z^{2L_0} - 1} = -\frac{1}{2\pi i} \int_{\bar{\Gamma}} \frac{dz}{z} \frac{g(z, x_0)}{e^{iL_0\phi} z^{2L_0} - 1} , \quad (\text{D.11})$$

where the contour $\hat{\Gamma}$ encircles the poles \hat{z}_ℓ but not the poles \bar{z}_i , while for $\bar{\Gamma}$ it is the other way around. Since

$$\text{Res} \left(\frac{1}{z} \frac{1}{\omega^2 - (z - z^{-1})^2} \right)_{z=\bar{z}_i} = \frac{1}{2(1/\bar{z}_i^2 - \bar{z}_i^2)} , \quad (\text{D.12})$$

then

$$\Sigma(x_0) = -\frac{1}{2} \sum_{i=1}^4 \frac{\bar{z}_i^{2x_0}}{e^{iL_0\phi} \bar{z}_i^{2L_0} - 1} \frac{1}{1/\bar{z}_i^2 - \bar{z}_i^2} . \quad (\text{D.13})$$

By setting $\omega = 2 \sinh(\hat{\omega}/2)$, it then follows that $\bar{z}_i^2 = e^{\pm \hat{\omega}}$ and

$$\Sigma(x_0) = \frac{1}{2 \sinh \hat{\omega}} \left[\frac{e^{\hat{\omega}x_0}}{e^{iL_0\phi+L_0\hat{\omega}} - 1} - \frac{e^{-\hat{\omega}x_0}}{e^{iL_0\phi-L_0\hat{\omega}} - 1} \right] . \quad (\text{D.14})$$

The real and imaginary parts read

$$\text{Re } \Sigma(x_0) = \frac{\sinh(L_0\hat{\omega}/2) \cosh[\hat{\omega}(L_0/2 - x_0)] - \sin^2(L_0\phi/2) \sinh(\hat{\omega}x_0)}{\sinh \hat{\omega} (\cosh(L_0\hat{\omega}) - \cos(L_0\phi))} , \quad (\text{D.15})$$

$$\text{Im } \Sigma(x_0) = \frac{-\sin(L_0\phi) \sinh(\hat{\omega}x_0)}{2 \sinh(\hat{\omega}) (\cosh(L_0\hat{\omega}) - \cos(L_0\phi))} . \quad (\text{D.16})$$

For $\phi = 0$, corresponding to periodic boundary conditions, one recovers the known (real) result

$$\Sigma(x_0) = \frac{1}{2 \sinh \hat{\omega}} \frac{\cosh[\hat{\omega}(L_0/2 - x_0)]}{\sinh(L_0\hat{\omega}/2)} . \quad (\text{D.17})$$

Finally the propagator is obtained by inserting Eq. (D.14) in Eq. (D.1) for each value of \mathbf{p} after having made the substitutions in Eq. (D.3).

D.1 Expectation value of T_{0k} for the $\text{SU}(N)$ gauge theory

We are interested in the expectation value of the momentum density operator in the non-interacting limit of the $\text{SU}(N)$ gauge theory in presence of shifted boundary conditions. We discretize T_{01} using the ‘clover’ discretization of the field strength tensor as described in [19, 20]. Using the perturbative expansion and taking the infinite volume limit we obtain [20]

$$\begin{aligned} \frac{1}{2(N^2 - 1)} \langle T_{01} \rangle &= \frac{1}{L_0} \sum_{\ell=0}^{L_0-1} \int_{BZ} \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{\sin(2\pi\ell/L_0 - \mathbf{p} \cdot \boldsymbol{\xi}) \cos^2(p_2/2) \sin(p_1)}{4 \sin^2(\frac{\pi\ell}{L_0} - \frac{\mathbf{p} \cdot \boldsymbol{\xi}}{2}) + 4 \sum_{k=1}^3 \sin^2(p_k/2)} \\ &= \int_{BZ} \frac{d^3\mathbf{p}}{(2\pi)^3} \cos^2(p_2/2) \sin(p_1) \text{Im } \Sigma(1) , \end{aligned} \quad (\text{D.18})$$

where in the latter equation for $\Sigma(1)$ we use Eq. (D.16) with $\omega^2 = 4 \sum_{k=1}^3 \sin^2(p_k/2)$ and $\phi = \mathbf{p} \cdot \boldsymbol{\xi}$. The three-dimensional integral in Eq. (D.18) can be evaluated numerically leading to Fig. 1.

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